Web Technologies for Bioinformatics

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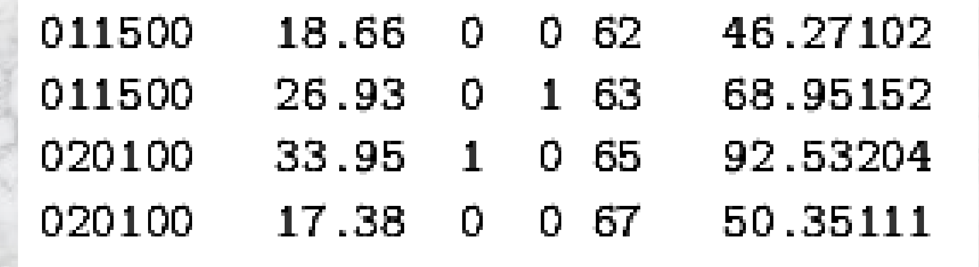
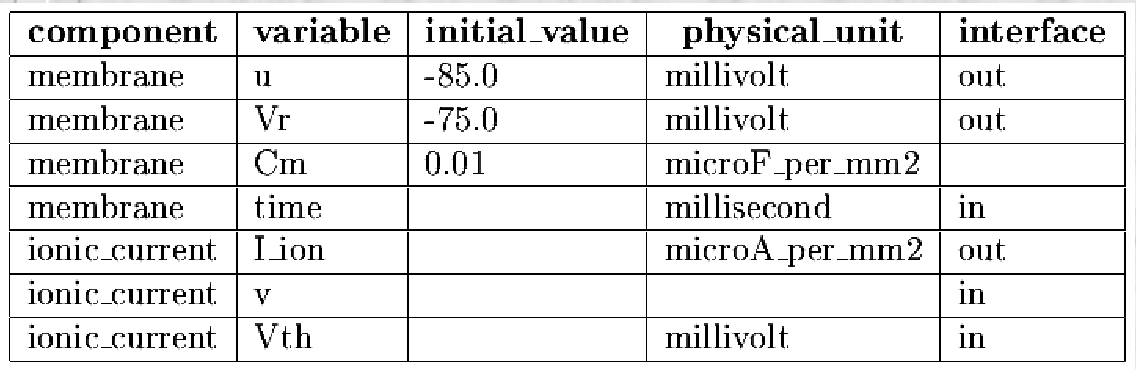
Data Formats

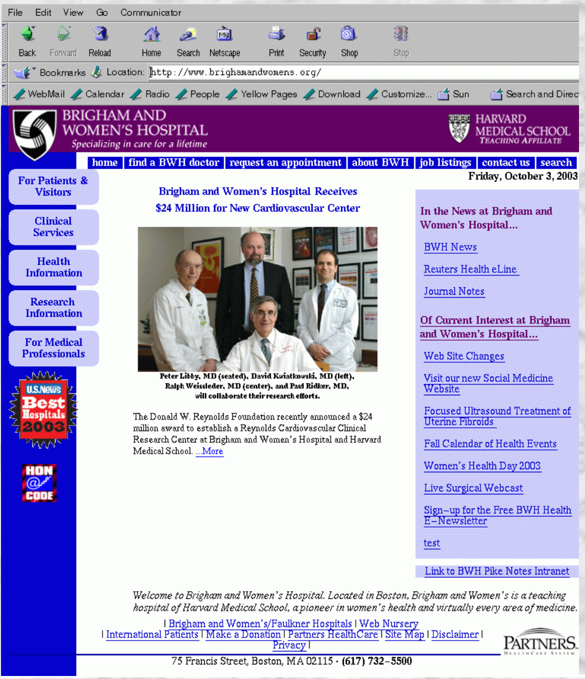
- Flat files
- Spreadsheets
- Relational databases
- Web sites



```
011500    18.66  0  0 62    46.27102
011500    26.93  0  1 63    68.95152
020100    33.95  1  0 65    92.53204
020100    17.38  0  0 67    50.35111
```



component	variable	initial_value	physical_unit	interface
membrane	u	-85.0	millivolt	out
membrane	Vr	-75.0	millivolt	out
membrane	Cm	0.01	microF_per_mm2	
membrane	time		millisecond	in
ionic_current	I_ion		microA_per_mm2	out
ionic_current	v			in
ionic_current	Vth		millivolt	in



Friday, October 3, 2003

Brigham and Women's Hospital Receives
$24 Million for New Cardiovascular Center

Peter Libby, MD (seated), David Kwiatkowski, MD (left), Ralph Weissleder, MD (center), and Paul Ridker, MD, will collaborate their research efforts.

The Donald W. Reynolds Foundation recently announced a $24 million award to establish a Reynolds Cardiovascular Clinical Research Center at Brigham and Women's Hospital and Harvard Medical School. ...More

In the News at Brigham and Women's Hospital...

BWH News

Reuters Health eLine

Journal Notes

Of Current Interest at Brigham and Women's Hospital...

Web Site Changes

Visit our new Social Medicine Website

Focused Ultrasound Treatment of Uterine Fibroids

Fall Calendar of Health Events

Women's Health Day 2003

Live Surgical Webcast

Sign–up for the Free BWH Health E–Newsletter

test

Link to BWH Pike Notes Intranet

Welcome to Brigham and Women's Hospital. Located in Boston, Brigham and Women's is a teaching hospital of Harvard Medical School, a pioneer in women's health and virtually every area of medicine.

| Brigham and Women's/Faulkner Hospitals | Web Nursery
| International Patients | Make a Donation | Partners HealthCare | Site Map | Disclaimer |
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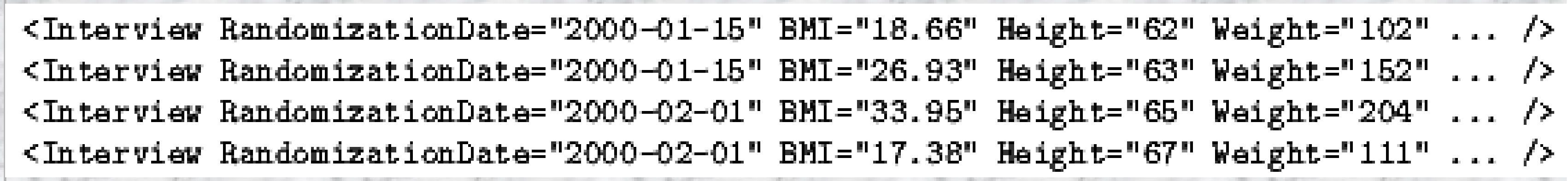
XML Documents

- Flexible very popular text format
- Self-describing records



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<Interview RandomizationDate="2000-01-15" BMI="18.66" Height="62" Weight="102" ... />
<Interview RandomizationDate="2000-01-15" BMI="26.93" Height="63" Weight="152" ... />
<Interview RandomizationDate="2000-02-01" BMI="33.95" Height="65" Weight="204" ... />
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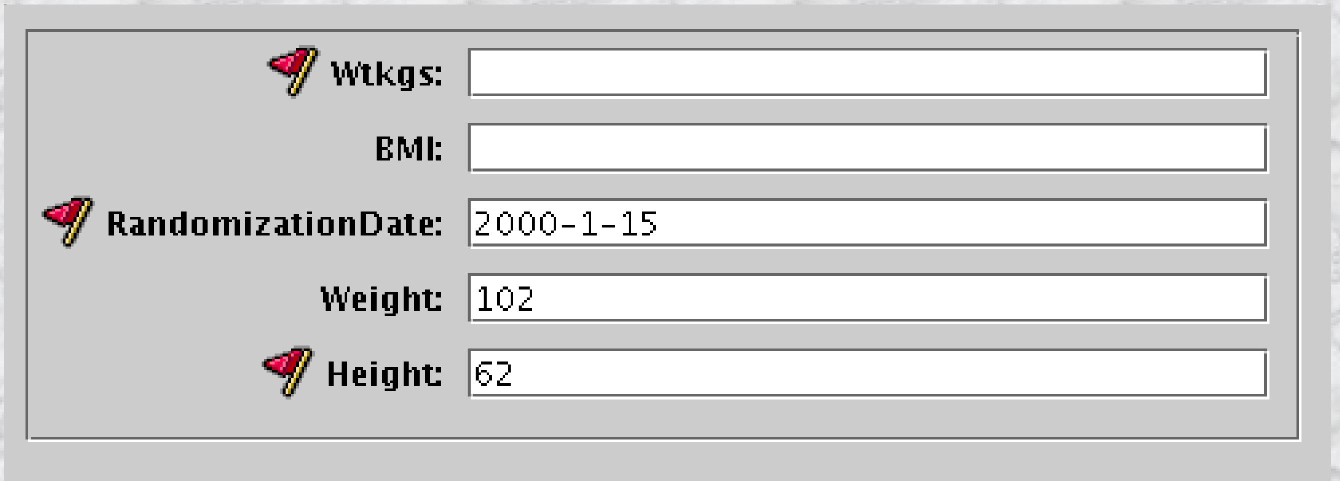
```



Wtkgs:

BMI:

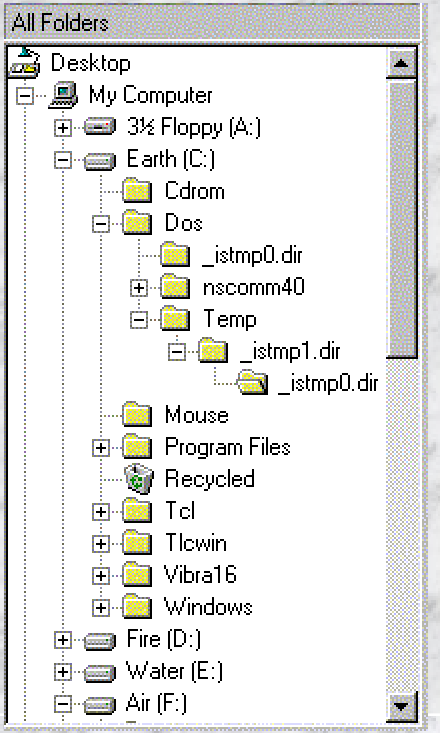
RandomizationDate: 2000-1-15

Weight: 102

Height: 62

XML Documents (continued)

- Hierarchical structure



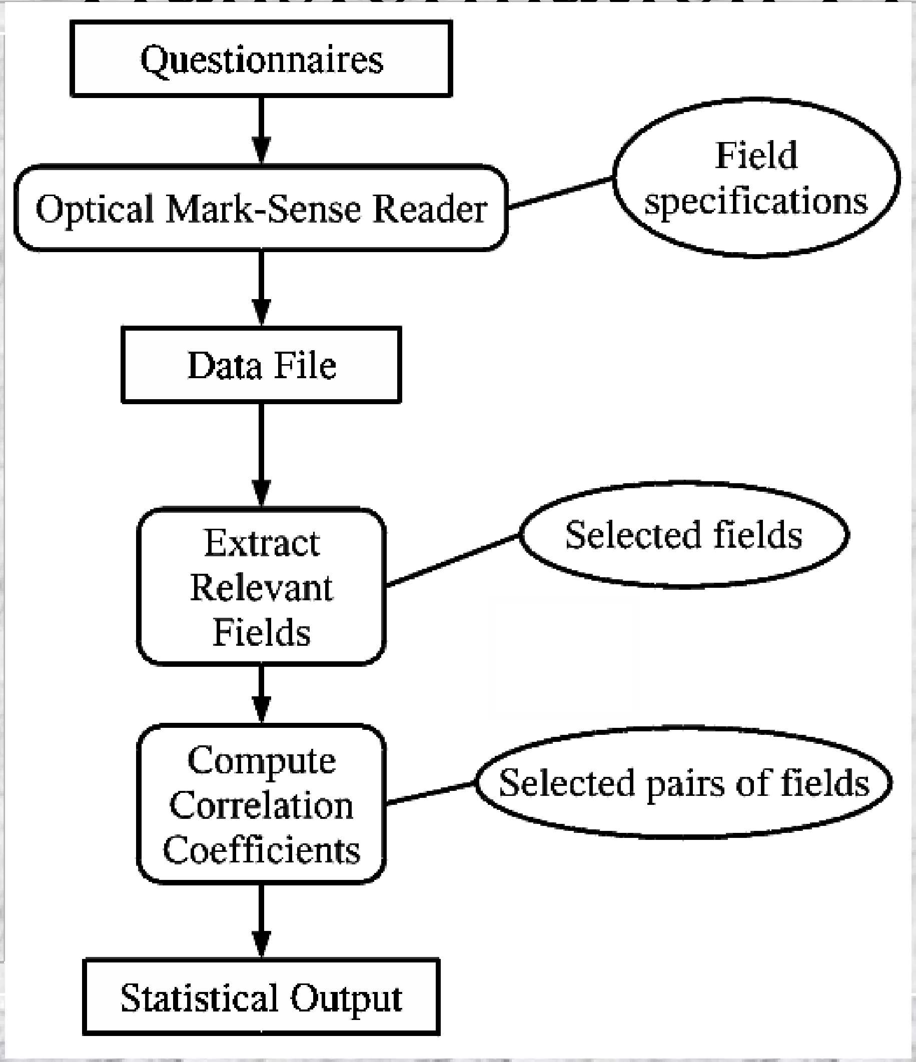
All Folders

```
Desktop
  My Computer
    3½ Floppy (A:)
    Earth (C:)
      Cdrom
      Dos
        _istmp0.dir
        nscomm40
        Temp
          _istmp1.dir
            _istmp0.dir
      Mouse
      Program Files
      Recycled
      Tcl
      Tlcwin
      Vibra16
      Windows
    Fire (D:)
    Water (E:)
    Air (F:)
```

Purpose of Data

- Data is collected and stored for a purpose.
- The format serves that purpose.
- Using data for another purpose is common.
- Data presentation (such as on a Web site) is one example of such a use.
- It is important to anticipate that data will be used for many purposes.
- Data is reused by *transforming* it.

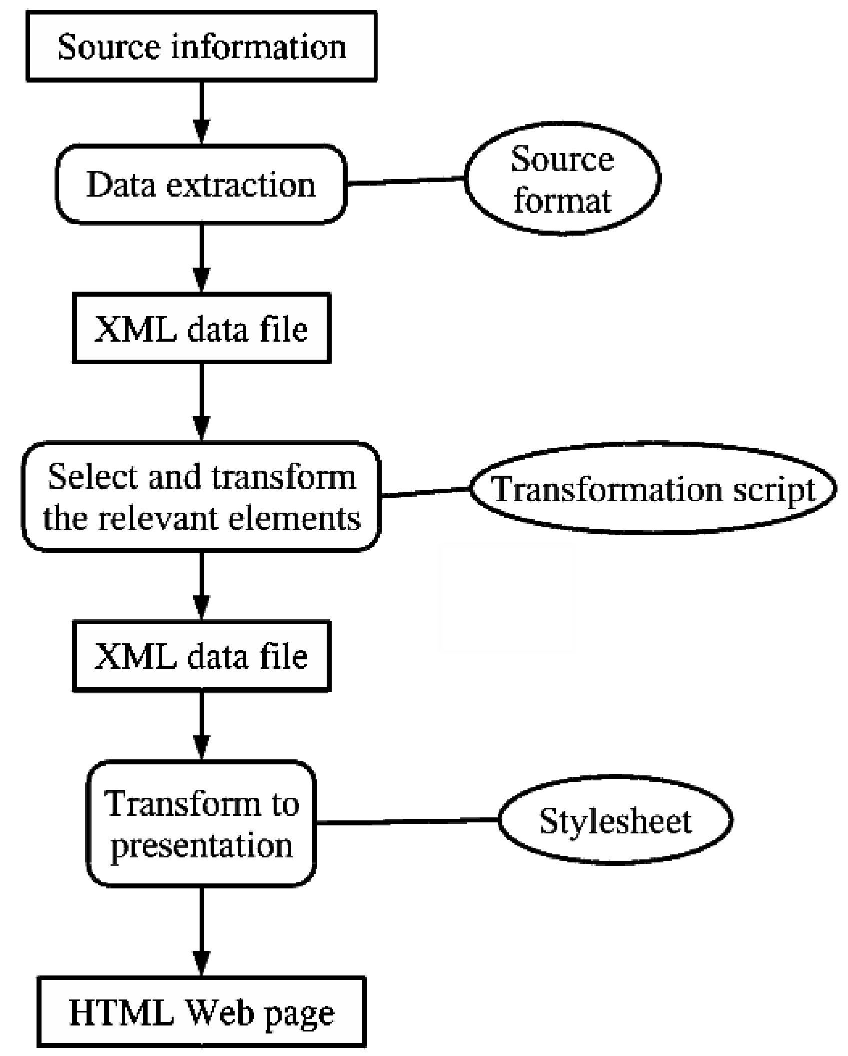
Statistical Analysis as a Transformation Process



- Transformation consists of a series of steps.
- Specialized equipment and software is used for each step.
- Separation into steps reduces the overall effort.

Web Site Construction

- Web sites can be constructed using a Web site authoring tool (e.g., Front Page).
- Alternatively, one could use a transformation process to separate concerns.



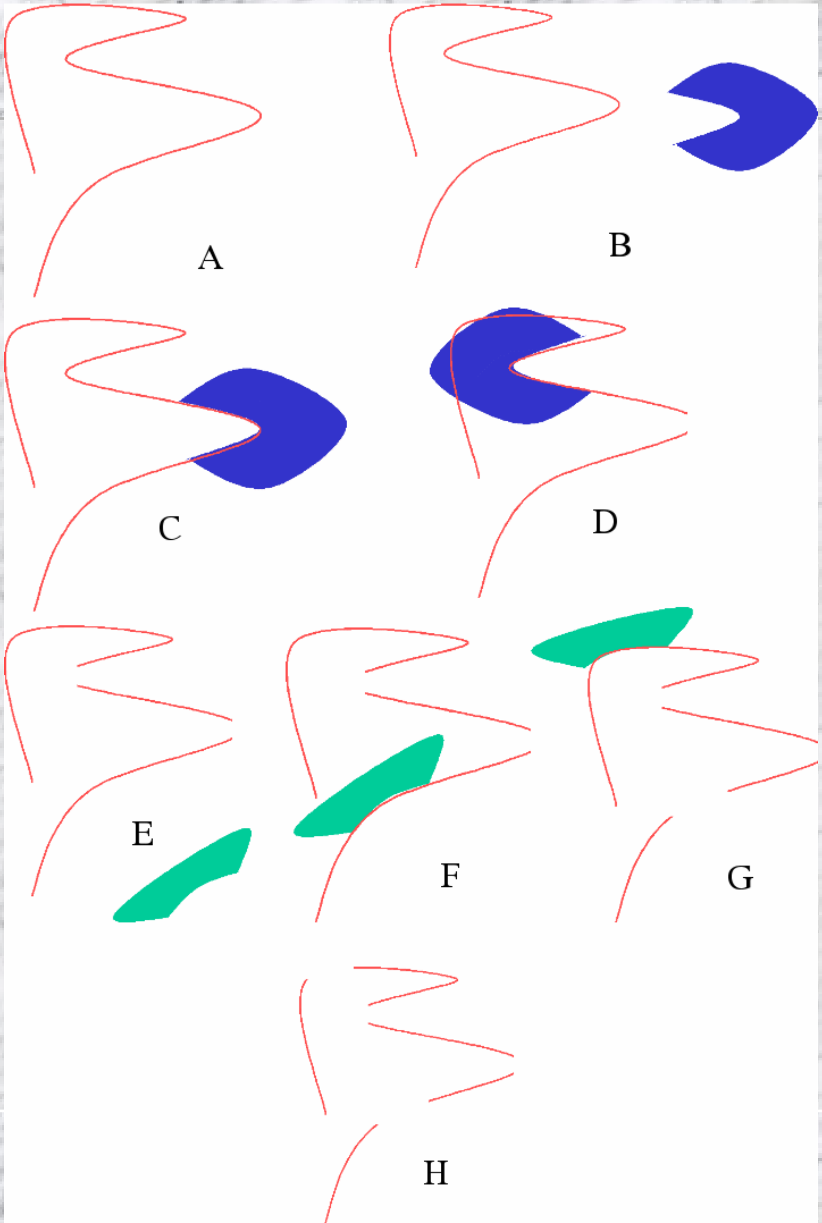
Advantages of Transformation

- Reduces the overall effort.
- Presentation style is independent of the source content.
- Presentation style can be changed with immediate effect.
- Uniform enforcement of presentation style.
- Updates to content are immediate.
- Content can be used for many other purposes:
  - **Many reports in many formats**
  - **Proposals**
  - **Data sharing with other institutions**
  - **Data mining**

Transformation Languages

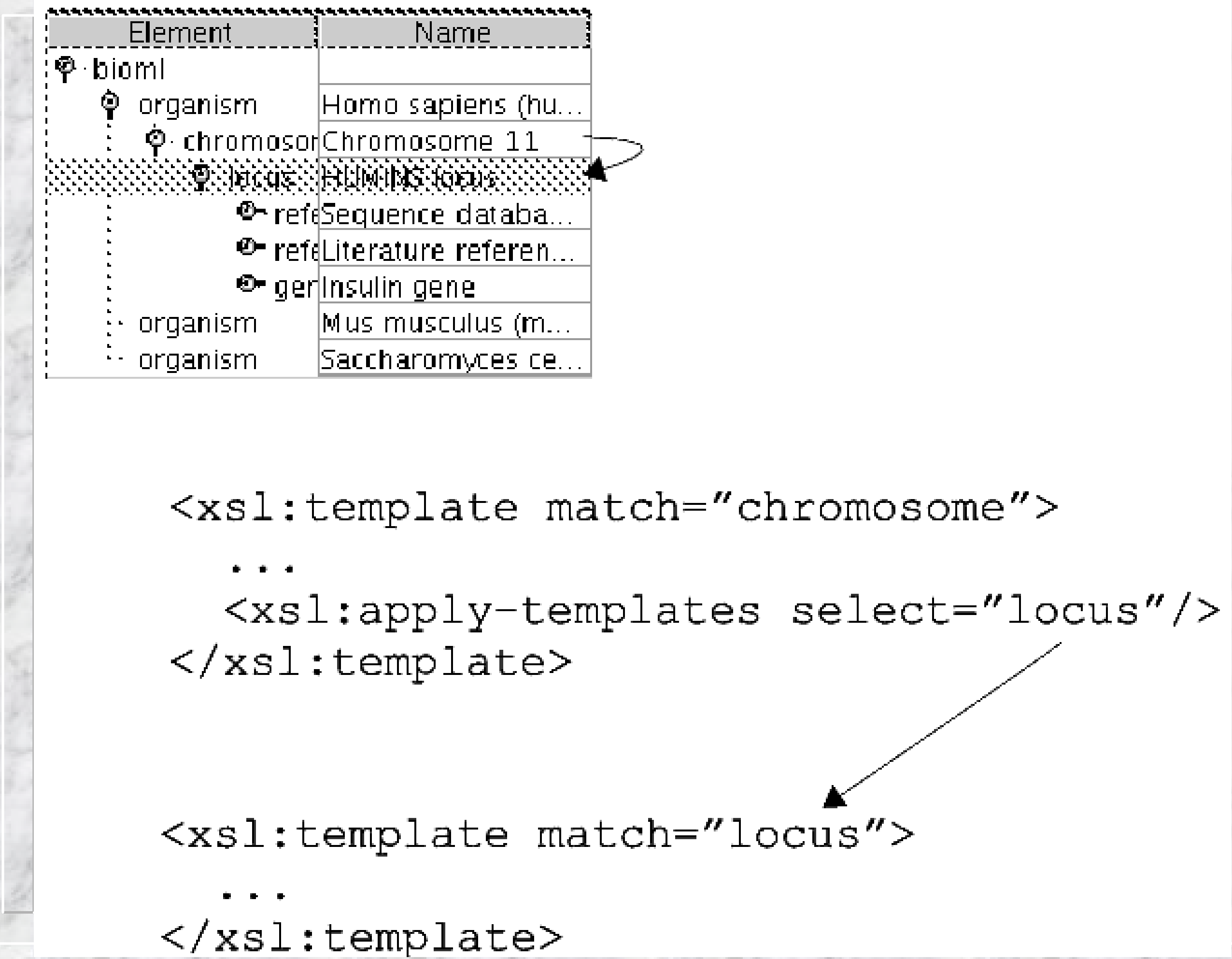
- Traditional programming languages such as Perl, Java, etc.
- Rule-based (declarative) languages such as the XML Transformation language (XSLT).
  - Rule-based rather than procedural
  - Transform each kind of element with a template
  - Matching and processing of elements is analogous to the digestion of polymers with enzymes.

Transformation as Digestion



- The blue enzyme attacks the polymer at two locations.
- The resulting three polymers are then attacked by the green enzyme.

XSLT “Digestion”



Element	Name
bioml	
organism	Homo sapiens (hu…
chromosor	Chromosome 11
locus	HUMINS locus
refe	Sequence databa…
refe	Literature referen…
ger	Insulin gene
organism	Mus musculus (m…
organism	Saccharomyces ce…

```
<xsl:template match=”chromosome”>
   ...
   <xsl:apply-templates select=”locus”/>
</xsl:template>


<xsl:template match=”locus”>
   ...
</xsl:template>
```

- An XSLT program consists of templates
- Each template processes a set of matching elements
- A template can break up the element to be processed by other templates

```
<?xml version="1.0"?>
<xsl:transform version="1.0”
 xmlns:xsl="http://www.w3.org/1999/XSL/Transform">

<!-- Change all occurrences of P to Protein -->
<xsl:template match="P">
  <Protein>
    <xsl:apply-templates select="@*|node()"/>
  </Protein>
</xsl:template>

<!-- Change all occurrences of S to Substrate -->
<xsl:template match="S">
  <Substrate>
    <xsl:apply-templates select="@*|node()"/>
  </Substrate>
</xsl:template>

<!-- Don't change anything else -->
<xsl:template match="@*|node()">
  <xsl:copy>
    <xsl:apply-templates match="@*|node()"/>
  </xsl:copy>
</xsl:template>

</xsl:transform>
```

```
<Array><P id="Mas375"><interactionsubstrate="Sub89032">
<BindingStrength>5.67</BindingStrength><Concentration
unit="nm">43</Concentration></interaction><interaction
substrate="Sub89033"><BindingStrength>4.37</BindingStrength>
<Concentration unit="nm">75</Concentration></interaction></P><P
id="Mtr245"><interaction substrate="Sub89032">
<BindingStrength>0.65</BindingStrength><Concentration
unit="um">0.53</Concentration></interaction><interaction
substrate="Sub80933"><BindingStrength>8.87</BindingStrength>
<Concentration
unit="nm">8.4</Concentration></interaction></P><S
id="Sub89032"/><S id="Sub89033"/></Array>
```

```xml
<Array>
   <Protein id="Mas375">
      <interaction substrate="Sub89032">
         <BindingStrength>5.67</BindingStrength>
         <Concentration unit="nm">43</Concentration>
      </interaction>
      <interaction substrate="Sub89033">
         <BindingStrength>4.37</BindingStrength>
         <Concentration unit="nm">75</Concentration>
      </interaction>
   </Protein>
   <Protein id="Mtr245">
      <interaction substrate="Sub89032">
         <BindingStrength>0.65</BindingStrength>
         <Concentration unit="um">0.53</Concentration>
      </interaction>
      <interaction substrate="Sub80933">
         <BindingStrength>8.87</BindingStrength>
         <Concentration unit="nm">8.4</Concentration>
      </interaction>
   </Protein>
   <Substrate id="Sub89032"/>
   <Substrate id="Sub89033"/>
</Array>
```

Ontologies

- The structure of data is its ontology.
  - Database schema
  - XML Document Type Definition (DTD)
- An ontology defines the concepts and relationships between them in a domain.
- Transformations are fundamental:
  - Queries
  - Organizing data (views)
  - Transformation for new purposes

Research Areas

- Ontologies for bioinformatics
- Ontology development in general
  - Constructing ontologies
  - Validation and testing of ontologies
- New ontology languages to capture more meaning
- Transformation languages

Research Areas

- Inference and deduction
  - Logical inference
  - Probabilistic inference
  - Scientific inference
  - Other forms of inference
- Integrating inference with
  - Data mining
  - Experimental processes